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Rev	Date	Description of Change(s)	Preparer	Verifier	RM	FDAR
0	3/10/2021	Original Issue	Yong Tao	Jacob Riglin	Chris James	Jorge Ruiznavarro
1	4/20/2021	Revision 1 Calculations are revised to add Appendix A, Estimation of filter media instant surface temperature.	Yong Tao 316341 YONG TAO (Affiliate) Digitally signed by YONG TAO (Affiliate) Date: 2021.05.18 12:34:55 -06'00'	Phil Hypes 153911 PHILIP HYPES (Affiliate) Digitally signed by PHILIP HYPES (Affiliate) Date: 2021.05.21 08:16:52 -06'00'	Phil Hypes 153911 PHILIP HYPES (Affiliate) Digitally signed by PHILIP HYPES (Affiliate) Date: 2021.05.21 08:17:11 -06'00'	Jorge Ruiznavarro 136928 JORGE CEREIJO RUIZNAVARRO (Affiliate) Digitally signed by JORGE CEREIJO RUIZNAVARRO (Affiliate) Date: 2021.05.20 15:11:41 -06'00'

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1.0 PURPOSE

This calculation documents the estimation of temperature and pressure rise inside a 55-gal TRU waste drum with a HEPA filter containing Titanium and Tantalum fume dust based on operational history. Actual Titanium values are believed to be less than 10g on any given filter. Actual Tantalum values are believed to be less than 1g on any given filter.

On 2/26/2021 an energy release event occurred during waste bagout. Two bagged HEPA filters (one standing open-face media up) and a spacer were in the drum. The bags may have preserved an inert Argon atmosphere around the filters. An empty, lidless con-flat container was dropped onto the filter media. This caused a loud noise and a quick shower of sparks, reddish orange in color. The HEPA filters in question were the Flanders model number is 0-007-D-43-R0-Nu-00-00-Z93555H 8" inch diameter, 5.875" depth, borosilicate filter media, nuclear grade HEPA filters, stainless steel clad type. The estimated HEPA filter weight is 5 to 7 lb. The Process Status code was AO (Assembly Operation). The filter media of the HEPAs was very dark in color.

The initial investigation found there were very low levels of radioactive material on the filters. It was conjectured that dropping the con-flat container onto the bagged filters violated the bags, allowing oxygen into the filters, and adding energy to the system. This caused rapid oxidation of Titanium and Tantalum fume dust collected on the HEPA filter from laser welding process.

This calculation estimates the possible maximum pressure rise caused by the rapid oxidation of Titanium and Tantalum fume dust collected on one HEPA filter.

2.0 METHODOLOGY

The possible Titanium and Tantalum fume dust loading on the HEPA filter was estimated based on the welding process (Ref. 6). The estimated masses of Titanium and Tantalum are listed in Table 1.

Table 1. Calculated masses of Ti and Ta on HEPA filters

Filter Change Date	2/19/2021	6/26/2020	1/18/2020	10/15/2019	2/10/2019	9/18/2018
Calculated mass of Ti fume, g	0.64	1.25	0.52	3.54	1.6	0.33
Calculated mass of Ta fume, g	0.08	0	0	0.01	0	0.18

The oxidation of Titanium and Tantalum can be described by the following equations:

$$Ti + O_2 \rightarrow TiO_2$$

$$4\,Ta + 5\,O_2 \rightarrow 2\,Ta_2O_5$$

The enthalpy of these reactions is gotten from literature. Then the pressure rise of the drum is calculated based on the energy released if these Titanium and Tantalum were rapidly oxidized at

the same time. The maximum amount of these metals that could be on a filter without over pressurizing a drum is also calculated.

3.0 ACCEPTANCE CRITERIA

N/A

There are no explicit acceptance criteria for this calculation.

4.0 UNVERIFIED ASSUMPTIONS

N/A.

5.0 ASSUMPTIONS

5.1 The weight of Flanders 8" diameter nuclear grade HEPA filter is about 5 to 7 lbs. The filter media is boron silicate fiber glass (https://www.aafintl.com/en/commercial/browse-products/commercial/hepa-ulpa-filters/hepa---nuclear-grade). 5 lbs (2270 g) weight is utilized in the calculation. This assumption is conservative. (Ref. 5)

5.2 Use the specific heat capacity of silicon dioxide (SiO_2), 0.740 J/g•K, as the specific heat capacity of HEPA filter.

5.3 Initial temperature is 298 K (25 °C).

5.4 Initial pressure is 11.2 psia (0.76 atm), the atmosphere pressure at Los Alamos. The results at 14.7 psia (1.0 atm) are also calculated.

5.5 The drum is adiabatic (heat loss is neglected). This assumption is conservative.

5.6 The drum is airtight (no gas loss). Therefore the volume of the air inside waste drum remains constant. This assumption is conservative.

5.7 Use the isochoric specific heat of air at 298 K, C_v = 20.78 J/mol•K in the calculation. Since the drum filter can vent and isochoric specific heat is lower than isobaric specific heat, this assumption is conservative.

5.8 Ideal gas law applies.

5.9 Titanium dioxide (TiO_2) and Ta_2O_5 are oxidation products. Titanium can form other suboxides such as TiO, Ti_2O_3 and Ti_3O_5 before it forms TiO_2. Even though the enthalpy of formation of Ti suboxides are high, the energy per mole of Ti will be less. TiO_2 is the highest bound oxide.

6.0 LIMITATIONS

N/A

7.0 CALCULATION INPUTS

CRC Handbook and Tables of Thermal Properties of Gases were used to obtain the required thermal properties of air and silicon dioxide. CRC Handbook and Jacob et al (2009) were used to obtain enthalpy values for the reactions.

8.0 COMPUTER HARDWARE AND SOFTWARE

N/A

9.0 SUMMARY AND CONCLUSIONS

Based on the estimation of Titanium and Tantalum mass (Table 1), we assume the drum contains one HEPA filter. The rapid oxidation of Titanium and Tantalum on HEPA filters will cause a maximum of 39 K temperature increase and 1.5 psig pressure increase. The pressure increase is less than the 14 psig seal failure value from DOE STD 5506-2007. Since the final temperatures are all below 100 °C, there is low risk of initiating combustion of any cheese cloth and plastic inside the drum (Ref. 7). The void volume inside the drum has little impact on the calculated temperature and pressure. This is due to the fact that HEPA filters absorb more heat than air does and the volume of air inside has less impact than the weight of HEPA filter has.

Assuming the drum is filled, has 104 L void volume, has one HEPA filter inside, and neglecting the heat absorption of other materials inside drum (a conservative assumption), 33.00 g Titanium is the maximum amount on the filter without over-pressurizing the drum; 115.59 g Tantalum is the maximum amount on the filter without over-pressurizing the drum.

Following are related temperature and pressure limits for TRU waste drum.

- DOE-STD-5506-2007 states seal failure occurs at about 14 psig.
- According to DOE-STD-5506-2007, 28 psig is the pressure to cause lid loss in a rapidly rising catastrophic physical ejection during a fire event.

For TRU waste drum containing combustible materials, document C-CDE-17-001 (Ref. 7) highlights an experimental analysis that was done to characterize the temperature at which cheesecloth ignites. The conclusion was that the onset of mass loss of untreated cheesecloth occurred at 282 °C to 313 °C.

Compare to the above limits, the calculated temperature and pressure in this calculation are much less.

Since the calculation neglects the heat absorption of other materials inside the drum, the heat loss, the latent heat of melting of metals and plastic, and gas release through the filter, the calculation is conservative.

10.0 REFERENCES

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11.0 CALCULATION

11.1 Assume drum only has one HEPA filter

Assume a 55-gallon (208 L) drum only has one Flanders 8-inch HEPA round filter inside. It is unlikely that a drum will contain solely one HEPA filter, however there is no known, consistent proportion of the drum volume occupied with other waste. Therefore for simplicity this calculation assumes the 208 L is occupied by air and one 8-inch HEPA round filter. The packing volume of the 8-inch round HEPA filter is 4.84 L. However, the filter media is porous. Therefore, the real material volume of the HEPA filter is much less than 4.84L. In this case, the volume of the HEPA filter can be neglected in the calculation. We have performed the calculation below for several actual and theoretical embedded titanium mass values.

1. Enthalpy of reactions

   According to CRC handbook and Jacob et al., at 298 K, the enthalpy of formation of TiO_2 is -944 kJ/mol and the enthalpy of formation of Ta_2O_5 is -2038 kJ/mol (exothermal reactions).

2. Heat generated

   $Q = m_{Ti} \div 47.87$ g/mol X 944 kJ/mol + $m_{Ta} \div 181$ g/mol X 0.5 X 2038 kJ/mol

3. Temperature increase

   The specific heat capacity of dry air is $C_{v,\,air} = 20.78$ J/mol•K
   At standard condition (273 K, 1 atm), the volume of 1 mole air is 22.4 L.
   At 298 K and 7,300 feet elevation (0.76 atm) at Los Alamos, the volume of 1 mole air is 32.2 L.
   The number of moles of dry air in the drum is n=208/32.2 = 6.46 mol

   The specific heat capacity of a HEPA filter (silicon dioxide) is $C_{p,\,HEPA} = 0.740$ J/g•K
   The mass of HEPA filter is m = 2270 g

   Temperature increase is
   $\Delta T = Q/(C_{p,\,HEPA} \bullet m + C_{v,\,air} \bullet n)$
   Final temperature $T_2 = 298 + \Delta T$
   Final temperature in Celsius $T_{2,c} = T_2 - 273$

4. Pressure increase

   Using ideal gas law

$$\frac{P_1 V_1}{T_1} = \frac{P_2 V_2}{T_2}$$

$$V_1 = V_2$$

$$P_2 = \frac{P_1 T_2}{T_1}$$

The pressure increase is $\Delta P = P_2 - P_1$

Table 2 lists the calculated results

Table 2 Calculated Temperature and Pressure for 208 L Void Volume in Drum at 0.76 atm

Filter Change Date	2/19/21	6/26/20	1/20/20	10/15/19	2/10/19	9/18/18
Calculated Temperature increase, K	7	14	6	38.5	17	4
Final Temperature, K	305	312	304	337	315	302
Final Temperature, Celsius	32	39	31	64	42	29
Calculated Pressure increase, psig	0.3	0.5	0.2	1.4	0.7	0.2

5. At 1 atmosphere pressure

Because the atmosphere pressure at WIPP is different, the calculation results will be slightly different. In order to illustrate the impact of atmosphere pressure and elevation, the results at sea level (1.0 atm) are calculated according to the method described above (1-4).

At 298 K and 1.0 atm at sea level, the volume of 1 mole air is 24.5 L.
The initial pressure is 1.0 atm (14.7 psia).

Table 3 listed the calculation results at 1.0 atm.

Table 3 Calculated Temperature and Pressure for 1 atm (208 L Void Volume)

Filter Change Date	2/19/21	6/26/20	1/20/20	10/15/19	2/10/19	9/18/18
Calculated Temperature increase, K	7	13	6	38	17	4
Final Temperature, K	305	311	304	336	315	302
Final Temperature, Celsius	32	38	31	63	42	29
Calculated Pressure increase, psig	0.3	0.7	0.3	1.9	0.8	0.2

The atmospheric pressure at sea level is higher than the atmospheric pressure at Los Alamos. This means 1 mole of air at sea level has less volume than 1 mole of air at Los Alamos. Therefore, there is more air in the drum at the same void volume. More air absorbs more heat. So, the calculated temperature rise at WIPP will be a little bit lower than the calculated temperature rise at Los Alamos. Because the initial pressure increases, the calculated pressure increase will be a little bit higher. The influence of atmosphere pressure is very small.

11.2 **Assume drum is filled and has one HEPA filter**

Assume a 55-gallon (208 L) drum is filled and has one 8-inch round HEPA filter inside. Although the drum is filled, there are significant void spaces between the materials inside. The average empty volume (air volume) of the 9 containers that may contain HEPA filters is estimated based

on the weight of the material inside. The estimated void volume is 180 L. Assume only the HEPA filter and air absorb the heat released from Titanium and Tantalum oxidation, and neglect the heat absorption of other materials inside drum. This is a conservative assumption. Assume there are no other adverse reactions inside the drum.

1. Enthalpy of reactions

   Same as 11.1.

2. Heat generated

   Same as 11.1

3. Temperature increase

   The number of moles of dry air in the drum is n = 180/32.2 = 5.59 mol

   Temperature increase is
   $\Delta T = Q/(C_{p,\,HEPA} \bullet m + C_{v,\,air} \bullet n)$
   Final temperature $T_2 = 298 + \Delta T$
   Final temperature in Celsius $T_{2,c} = T_2 - 273$

4. Pressure increase

$$P_2 = \frac{P_1 T_2}{T_1}$$

   The pressure increase is $\Delta P = P_2 - P$
   Table 4 list the calculation results

Table 4 Calculated Temperature and Pressure for 180 L Void Volume in Drum

Filter Change Date	2/19/21	6/26/20	1/20/20	10/15/19	2/10/19	9/18/18
Calculated Temperature increase, K	7	14	6	39	18	4
Final Temperature, K	305	312	304	337	316	302
Final Temperature, Celsius	32	39	31	64	43	29
Calculated Pressure increase, psig	0.3	0.5	0.2	1.5	0.7	0.2

5. The impact of void volume.

Comparison of Table 4 and Table 2 shows that the difference between 208L results and 180 L results is minimal. This is due to the fact that HEPA filters absorb more heat than air does and the volume of air inside has less impact than the weight of HEPA filter has. Table 5 shows the calculated results of the filter changed on 10/15/2019 at different void volumes. The results vary by 1% across the range of void volumes.

Table 5 Calculated Temperature and Pressure at different Void Volume

Filter Change Date	10/15/2019	10/15/2019	10/15/2019	10/15/2019
Void Volume, L	208	180	10	0.0001
Calculated Temperature increase, K	38.5	39	41	42
Final Temperature, K	336.5	337	339	340
Final Temperature, Celsius	64	64	66	67
Calculated Pressure increase, psig	1.4	1.5	1.6	1.6

11.3 The maximum amount of Ti or Ta that could be on a filter

The maximum amount of Titanium or Tantalum fume dust that could be on a filter without over pressurizing a drum is calculated based on 14 psig pressure rise inside 55-gallon drum. Assume the drum has 104 L void volume. This assumption is conservative. Assume only Titanium or Tantalum fume dust is on the HEPA filter.

1. Pressure increase

The pressure increase is 14 psig.
The final pressure is $P_{2,\,max}$ = 14 + 11.2 = 25.2 psia

2. Temperature increase

Using ideal gas law

$$\frac{P_1V_1}{T_1} = \frac{P_2V_2}{T_2}$$

$$V_1 = V_2$$

$$T_2 = \frac{P_2T_1}{P_1}$$

$T_{2,\,max}$ = (25.2 psia × 298 K)/11.2 psia = 671 K

ΔT_{max} = 671 – 298 = 373 K

3. Heat Generated

Q_{max} = ΔT_{max} × ($C_{p,\,HEPA}$•m + $C_{v,\,air}$•n)
= 373 K × (0.740 J/g•K ×2270 g + 20.78 J/mol•K ×3.23 mol)
= 650726 J
= 650.726 kJ

4. Maximum amount of Titanium

The enthalpy of formation of TiO_2 is 944 kJ/mol.

The maximum amount of Ti is:

$M_{Ti,max} = Q_{max} \div 944\ kJ/mol \times 47.87\ g/mol = 33.00\ g$

5. Amount of Tantalum

The enthalpy of formation of Ta_2O_5 is 2038 kJ/mol.

The maximum amount of Ta is:

$M_{Ta,max} = Q_{max} \div 2038\ kJ/mol \times 2 \times 181\ g/mol = 115.59\ g$

APPENDIX A Estimation of filter media instant surface temperature

1. Methodology

The instant temperature at the filter media surface is calculated based on the filter media active surface area S_{fm} = 10.04 ft^2 (Ref. 5). Assume Ti and Ta fume (Listed in Table 1) are evenly distributed on the filter media surface and the heat generated only dissipates into 1 millimeter depth of the filter media.

2. Assumptions

a) Assume Ti and Ta distribute evenly on filter media surface.
b) Assume all Ti and Ta are oxidized in 1 second. This assumption is conservative.
c) Assume heat dissipate depth is 0.1 cm (1 mm). Based on the heat generation rate and the thermal conductivity of filter media, this assumption is conservative. In order to simplify the calculation, heat dissipation depth d=0.1 cm is used.
d) The heat capacity of general glass 0.8 J/g.K is used as the heat capacity of filter media (ref. 8).
e) Assume the bulk density of filter media ρ= 0.347 g/cm^3. According to the Handbook of Glass properties (Ref. 8), the density of borosilicate glass is from 2.182 g/cm^3 to 1.843 g/cm^3. Because the filter media is made from borosilicate glass fiber and it is porous, it is assumed that the bulk density is 0.347 g/cm^3. This is an arbitrary assumption.

3. Calculation

a) The heat generated, Q, is calculated according to the method of 11.1 (step 1 and step 2).

b) The mass of filter media that instantly absorbs the heat.
The mass of tilter media that instantly absorbs heat is calculated based on the assumption c) and e).

$m_{fm} = S_{fm} \times d \times \rho = 10.04\ ft^2 \times 0.1\ cm \times 0.347\ g/cm^3 = 324\ g$

c) Instant surface temperature of filter media
Temperature increase is

$\Delta T_{fm} = Q / m_{fm} C_{p,fm}$
$C_{p,\,fm} = 0.8$ J/g.K
Instant surface temperature of filter media $T_{fm} = 298 + \Delta T_{fm}$
Instant surface temperature of filter media in Celsius $T_{fm,c} = T_{fm} - 273$

Table 6 shows the calculated results of the instant surface temperature of filter media.

Table 6 Calculated Instant Filter Media Surface Temperature.

Filter Change Date	2/19/2021	6/26/2020	1/18/2020	10/15/2019	2/10/2019	9/18/2018
Calculated mass of Ti fume, g	0.64	1.25	0.52	3.54	1.6	0.33
Calculated mass of Ta fume, g	0.08	0	0	0.01	0	0.18
Heat generated, J	13071	24650	10254	69865	31552	7521
Calculated Filter Media Instant Surface temperature, K	348	393	338	568	420	327
Calculated Filter Media Instant Surface temperature, ^{o}C	75	120	65	295	147	54

4. Discussions

Because this temperature is localized on the filter media surface, it doesn't directly contact with other materials inside waste drum. The filter media itself is borosilicate glass, which is noncombustible. Secondly, this calculated temperature is instantaneous temperature. It will decrease rapidly as heat is absorbed by the whole HEPA filter (including remaining filter media and the frame of HEPA filter). Therefore, it will not cause ignition problem inside the waste drum.